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Structure and Dynamics of Combustion Waves in Premixed Gases

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Lecture III
Thermal propagation of flames

Lecture 3: Thermal propagation

3-1. Quasi-isobaric approximation (Low Mach number)

3-2. One-step irreversible reaction

3-3. Unity Lewis number and large activation energy

3-4. Zeldovich & Frank-Kamenetskii asymptotic analysis

Preheated zone

Inner reaction layer

Matched asymptotic solution

3-5. Reaction diffusion waves

Phase space

Selected solution in an unstable medium

$III-1)$ Quasi-isobaric approximation. LowMach number

$$\rho(\mathbf{u}.\nabla)\mathbf{u} \approx -\nabla p \quad \Rightarrow \quad \delta p \approx \rho u \delta u$$

$$p \approx \rho a^2 \quad \Rightarrow \delta p/p \approx u^2/a^2 \equiv M^2 \quad \Leftarrow \delta u \approx u$$

slow evolution $\quad \partial/\partial t \approx \mathbf{u}.\nabla \ll a\,|\nabla|$

$+$ very subsonic flow $\quad M^2 \ll 1 \quad \Rightarrow \quad \delta p/p \ll \delta T/T = O(1)$

$$\frac{p}{\rho c_p T} = O(1)$$

$$\left|\frac{1}{p}\frac{\mathrm{D}p}{\mathrm{D}t}\right| \ll \left|\frac{1}{T}\frac{\mathrm{D}T}{\mathrm{D}t}\right| \quad \Rightarrow \quad \left|\frac{\mathrm{D}p}{\mathrm{D}t}\right| \ll \left|\rho c_p \frac{\mathrm{D}T}{\mathrm{D}t}\right|$$

$$\rho c_p \mathrm{D}T/\mathrm{D}t = \cancel{\mathrm{D}p/\mathrm{D}t} + \nabla.(\lambda\nabla T) + \sum_j Q^{(j)}\dot{W}^{(j)}$$

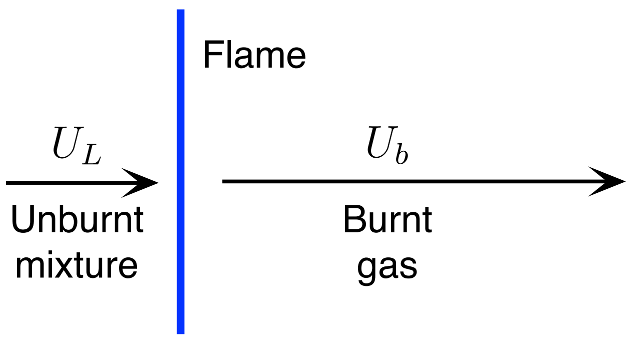
(in open space)

$$\rho T = \rho_o T_o$$

$$\rho c_p \mathrm{D}T/\mathrm{D}t = \nabla.(\lambda\nabla T) + \sum_j Q^{(j)}\dot{W}^{(j)}(T, ..Y_k..)$$

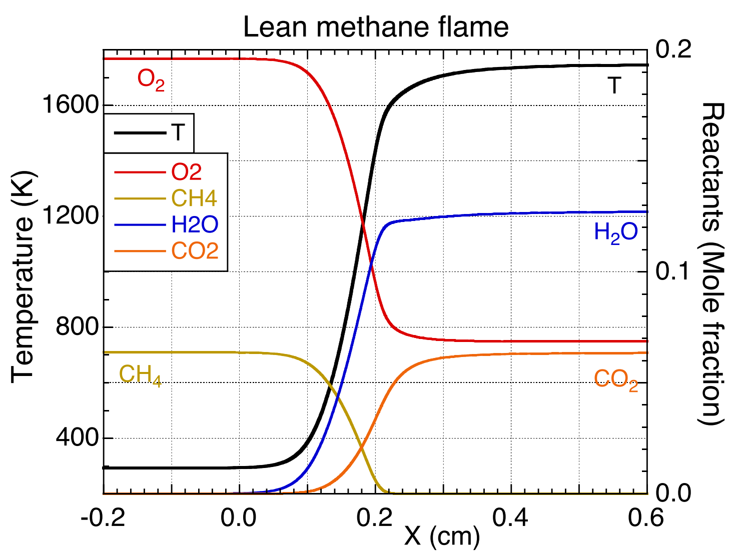
$$\rho \mathrm{D}Y_i/\mathrm{D}t = \nabla.(\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)} \mathsf{m}_i \dot{W}^{(j)}(T, ..Y_k..),$$

Planar flame reference frame of flame



$$\rho\, \mathrm{D/Dt} = m\mathrm{d}/\mathrm{d}x$$

$$m \equiv \rho_u U_L = \rho_b U_b, \qquad U_b/U_L \approx T_b/T_u, \approx 4-8$$



mass flux across the planar flame

quasi-isobaric approximation: $\rho T \approx \mathrm{cst.}$

equations

$$m c_p \frac{\mathrm{d}T}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\lambda \frac{\mathrm{d}T}{\mathrm{d}x}\right) = \sum_j Q^{(j)} \dot{W}^{(j)}(T, ..Y_i..)$$

$$m \frac{\mathrm{d}Y_i}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\rho D_i \frac{\mathrm{d}Y_i}{\mathrm{d}x}\right) = \sum_j \vartheta_i^{(j)} M_i \dot{W}^{(j)}(T, ..Y_{i'}..),$$

$m?$

boundary conditions

$$x = -\infty : \quad T = T_u, \ \ Y_i = Y_{iu}, \ \ \dot{W}^{(j)} = 0 \quad \text{frozen state}$$

$$x = +\infty : \ \ \mathrm{d}T/\mathrm{d}x = 0, \ \ Y_i = Y_{ib}, \ \ \dot{W}^{(j)} = 0 \quad \text{equilibrium state}$$

$III-2)$ One-step irreversible reaction

$$R \longrightarrow P + Q$$

R in an inert ; $\quad Y =$ mass fraction of R

Velocity and structure of the planar flame

$$mc_p\frac{\mathrm{d}T}{\mathrm{d}x}-\frac{\mathrm{d}}{\mathrm{d}x}\left(\lambda\frac{\mathrm{d}T}{\mathrm{d}x}\right)=\rho q_{_R}\dot{W}$$

$q_{_R} =$ energy released per unit of mass of R

$m \equiv \rho_u U_L$ unknown

$$m\frac{\mathrm{d}Y}{\mathrm{d}x}-\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho D\frac{\mathrm{d}Y}{\mathrm{d}x}\right)=-\rho\dot{W}$$

$$mY_u=\int_{-\infty}^{+\infty}\rho\dot{W}\,\mathrm{d}x$$

$x \to -\infty: \quad Y = Y_u,\ T = T_u$

$x \to +\infty: \quad Y = 0$

$$c_p(T_b-T_u)=q_m\equiv q_{_R}Y_u$$

Arrhenius law

$$\rho\dot{W}=\rho_b\frac{Y}{\tau_r(T)} \qquad \frac{1}{\tau_r(T)}\equiv\frac{\mathrm{e}^{-E/k_BT}}{\tau_{coll}} \qquad \frac{1}{\tau_{rb}}\equiv\frac{\mathrm{e}^{-E/k_BT_b}}{\tau_{coll}}$$

$$\frac{1}{\tau_r(T)}=\frac{1}{\tau_{rb}}\mathrm{e}^{-\frac{T_b}{T}\beta(1-\theta)} \qquad \beta\equiv\frac{E}{k_BT_b}\left(1-\frac{T_u}{T_b}\right) \qquad \theta\equiv\frac{T-T_u}{T_b-T_u}\in[0,1]$$

$III-3)$ Unity Lewis number and large activation energy

$\mathrm{Le} \equiv D_T/D$ Reduced temperature and mass fraction

$$\theta \equiv \frac{T-T_u}{T_b-T_u} \in [0,1] \qquad \psi \equiv \frac{Y}{Y_u} \in [0,1] \qquad \beta \equiv \frac{E}{k_B T_b}\left(1-\frac{T_u}{T_b}\right)$$

$$m\frac{\mathrm{d}\theta}{\mathrm{d}x} - \rho D_T \frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = \rho\frac{\dot{W}}{Y_{1u}}, \qquad m\frac{\mathrm{d}\psi}{\mathrm{d}x} - \frac{\rho D_T}{\mathrm{Le}}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\rho\frac{\dot{W}}{Y_{1u}}, \qquad \rho\frac{\dot{W}}{Y_u} = \rho_b\frac{\psi}{\tau_{rb}}\mathrm{e}^{-\frac{T_b}{T}\beta(1-\theta)}$$

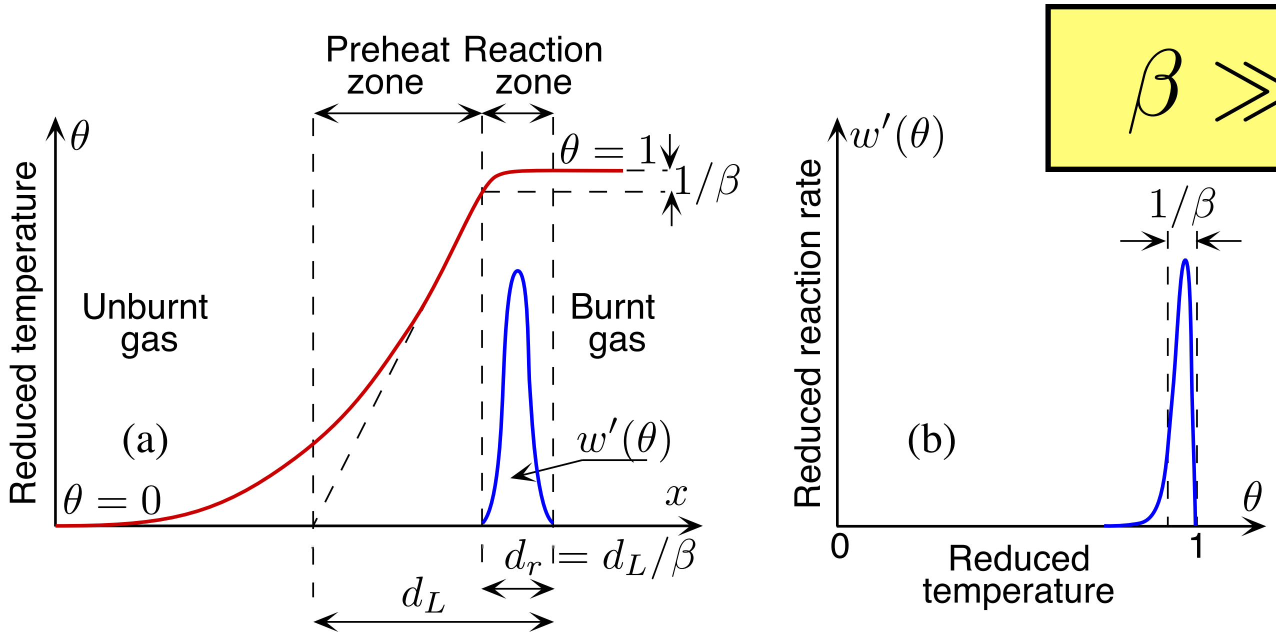
$$x=-\infty \ : \theta=0, \psi=1, \qquad x=+\infty \ : \theta=1, \psi=0$$

$$\mathrm{Le}=1$$

$$\psi = 1-\theta \qquad m\frac{\mathrm{d}\theta}{\mathrm{d}x} - \rho D_T \frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = \rho\frac{\dot{W}}{Y_{1u}}, \qquad \rho\frac{\dot{W}}{Y_u} = \rho_b\frac{(1-\theta)}{\tau_{rb}}\mathrm{e}^{-\frac{T_b}{T}\beta(1-\theta)}$$

$$x=-\infty \ : \theta=0, \qquad x=+\infty \ : \theta=1,$$

$$\beta \gg 1$$

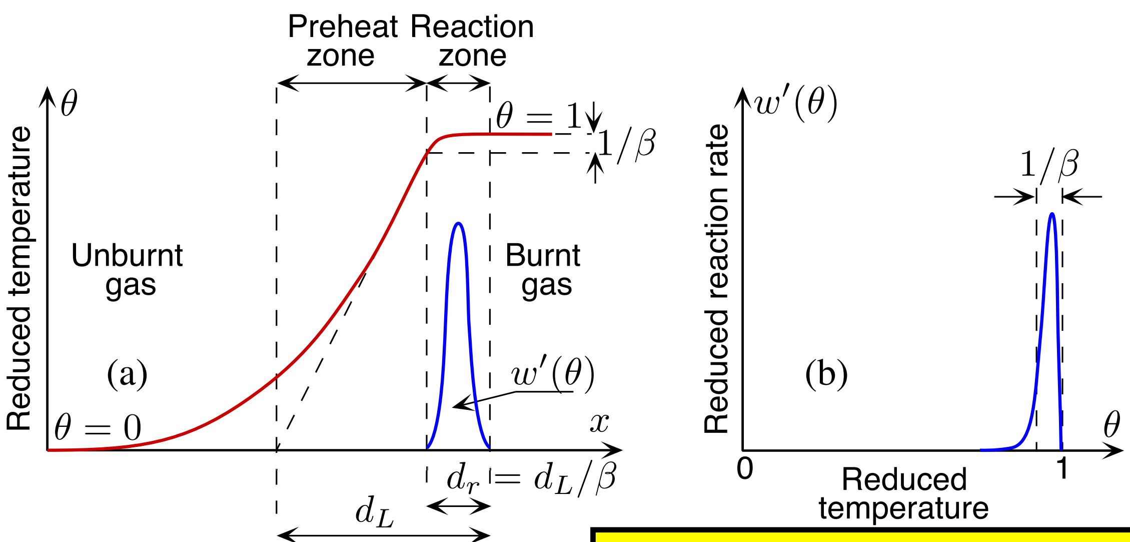


$$\rho\frac{\dot{W}}{Y_u} = \rho_b\frac{w'(\theta)}{\tau_{rb}}$$

$$w'(\theta) \approx (1-\theta)\mathrm{e}^{-\beta(1-\theta)}$$

(reaction rate is non negligible only when $T \approx T_b$)

$III-4)$ Zeldovich, Frank-Kamenetskii asymptotic analysis



$$\beta \longrightarrow \infty$$

Zeldovich 1938

$$m\frac{\mathrm{d}\theta}{\mathrm{d}x} - \rho D_T \frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} = \rho\frac{\dot{W}}{Y_{1u}},$$

$m?$

$x=-\infty \ : \theta=0, \qquad x=+\infty \ : \theta=1,$

$$w'(\theta) \approx (1-\theta)\mathrm{e}^{-\beta(1-\theta)}$$

$\rho\dot{W}/Y_u = \rho_b w'(\theta)/\tau_{rb}$

preheated zone $\dot{W}\approx 0$

$m\mathrm{d}\theta/\mathrm{d}x - \rho D_T \mathrm{d}^2\theta/\mathrm{d}x^2 = 0 \qquad \rho D_T = \text{cst.} \qquad \theta = \mathrm{e}^{mx/\rho D_T}$

origin $x=0$: location of the reaction zone $\theta=1$

$$d_L \equiv \rho D_T/m = D_{T_u}/U_L$$

matching condition

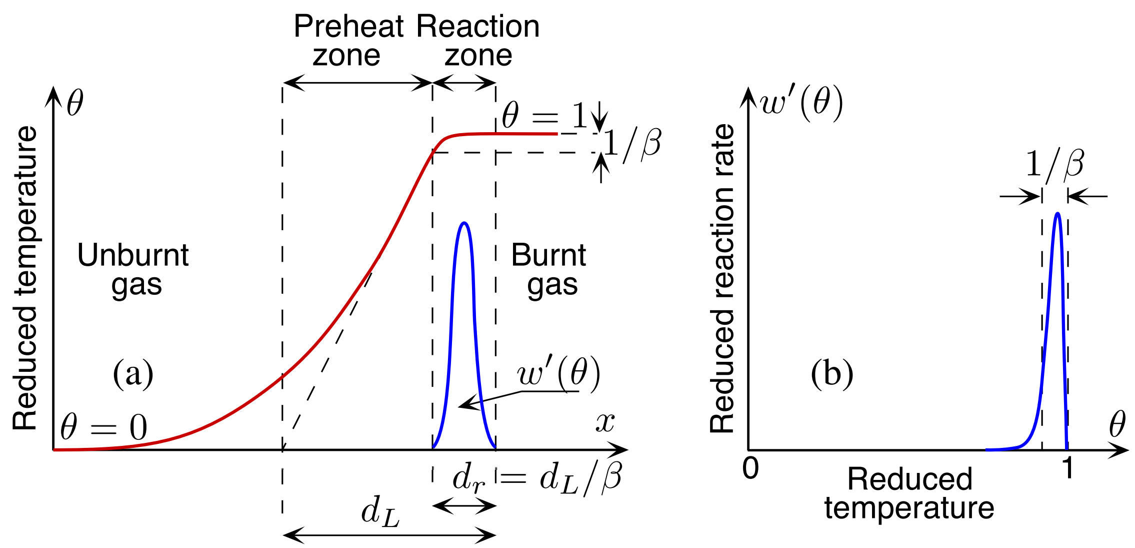
heat flux into the preheated zone

$$\rho D_T \mathrm{d}\theta/\mathrm{d}x|_{\theta=1} = m$$

should be equal to the heat flux from the thin reaction layer

Inner reaction layer

$$\boxed{1-\theta = O(1/\beta)} \qquad w'(\theta) \approx (1-\theta)\mathrm{e}^{-\beta(1-\theta)} = O(1/\beta)$$



$$m\frac{\mathrm{d}\theta}{\mathrm{d}x} \approx m\frac{\delta\theta}{d_r} \approx \frac{\rho_b D_{Tb}}{d_r d_L}\frac{1}{\beta} \Leftarrow \quad m = \rho D_T/d_L, \quad \delta\theta = O(1/\beta)$$

$$\rho_b D_{Tb}\frac{\mathrm{d}^2\theta}{\mathrm{d}x^2} \approx \rho_b D_{Tb}\frac{\delta\theta}{d_r^2} \approx \frac{\rho_b D_{Tb}}{d_r^2}\frac{1}{\beta}$$

$$\frac{\rho_b}{\tau_{rb}}w'(\theta) \approx \frac{\rho_b}{\tau_{rb}}\delta\theta \approx \frac{\rho_b}{\tau_{rb}}\frac{1}{\beta}$$

$$d_r \approx \sqrt{D_{Tb}\tau_{rb}} \qquad \boxed{d_r \ll d_L}$$

$$m\mathrm{d}\theta/\mathrm{d}x - \rho D_T \mathrm{d}^2\theta/\mathrm{d}x^2 = \frac{\rho_b}{\tau_{rb}}(1-\theta)\mathrm{e}^{-\beta(1-\theta)}$$

$$-\frac{D_{Tb}}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}\theta}{\mathrm{d}x}\right)^2 \approx \frac{1}{\tau_{rb}}(1-\theta)\mathrm{e}^{-\beta(1-\theta)}\frac{\mathrm{d}\theta}{\mathrm{d}x}$$

$$\Theta = \beta(1-\theta) \quad \Rightarrow \quad \tau_{rb}\frac{D_{Tb}}{2}\left(\frac{\mathrm{d}\theta}{\mathrm{d}x}\right)^2 \approx \int_\theta^1 (1-\theta)\mathrm{e}^{-\beta(1-\theta)}\mathrm{d}\theta = \frac{1}{\beta^2}\int_0^{\beta(1-\theta)} \Theta\mathrm{e}^{-\Theta}\mathrm{d}\Theta$$

Asymptotic solution $\beta \to \infty$

$$\int_0^\infty \Theta\mathrm{e}^{-\Theta}\mathrm{d}\Theta = 1$$

upstream exit of the inner layer $\quad \beta(1-\theta) \to \infty \;:\; D_{Tb}\mathrm{d}\theta/\mathrm{d}x \to \sqrt{(2/\beta^2)D_{Tb}/\tau_{rb}}$

downstream entrance of the external zone $\quad \theta \to 1 :\; \rho_b D_{Tb}\mathrm{d}\theta/\mathrm{d}x|_{\theta=1} = m$

matching

$$\boxed{m = \rho_b\sqrt{(2/\beta^2)D_{Tb}/\tau_{rb}},} \quad U_L = m/\rho_u, \Rightarrow \quad \boxed{d_r/d_L = O(1/\beta)}$$

$$U_L \approx \sqrt{D_{Tb}/\tau_{rb}}$$

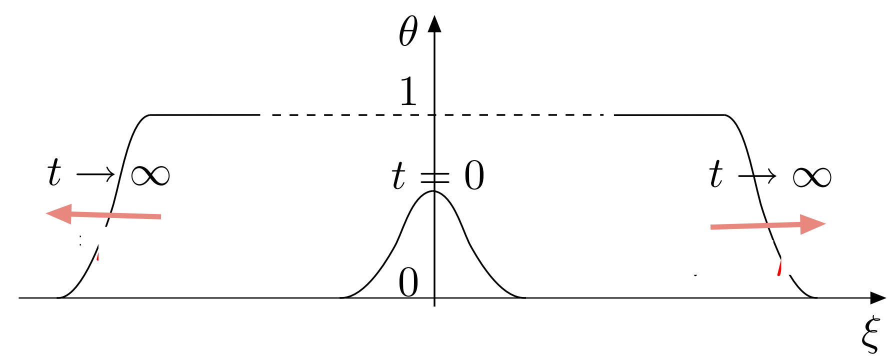
dimensional analysis

$III - 5)$ Reaction diffusion waves

non-dimensional form $\quad \dfrac{\partial\theta}{\partial t} - \dfrac{\partial^2\theta}{\partial x^2} = w(\theta) \qquad \theta \geq 0 \qquad \theta \in [0,1]$

propagation of steady state $\theta = 1$ into steady state $\theta = 0$

steady state: $\omega = 0$

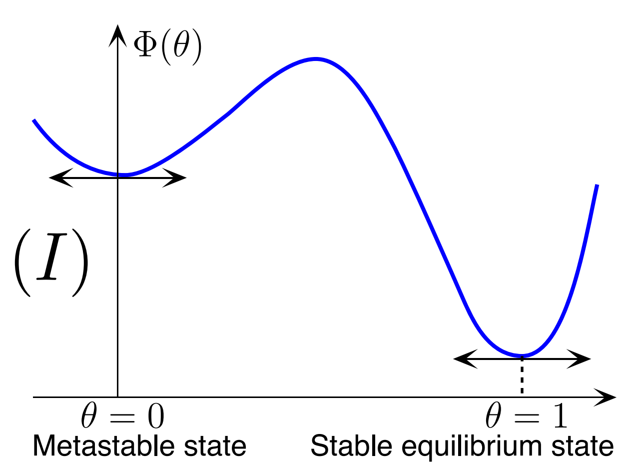


stability of steady states $\quad$ stable: $\mathrm{d}w/\mathrm{d}\theta < 0,$ unstable: $\mathrm{d}w/\mathrm{d}\theta > 0,$

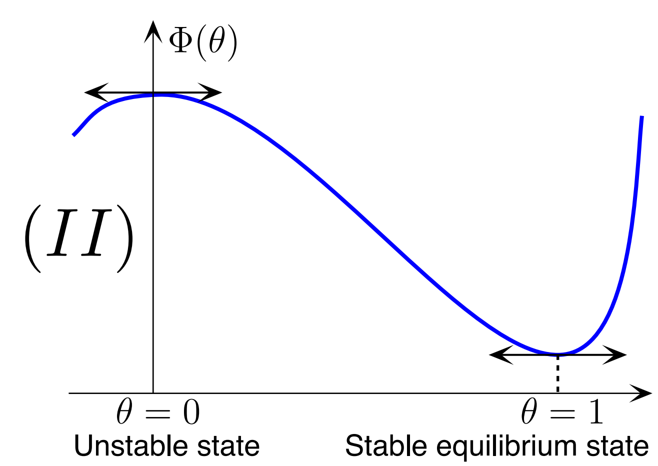
(equilibrium state) $\quad \theta = 1, \quad w = 0$ stable steady state

two different cases depending on the property of the initial state $\theta = 0$

initial state: $\quad (I): \quad \theta = 0, \quad w = 0$ metastable steady state (less stable)
$\qquad (II): \quad \theta = 0, \quad w = 0$ unstable steady state (out of equilibrium)



$$\mathrm{d}\Phi/\mathrm{d}\theta = -w(\theta)$$



propagating planar wave at constant velocity

$$\frac{\partial\theta}{\partial t} - \frac{\partial^2\theta}{\partial x^2} = w(\theta)$$ traveling wave solution (from right to left)

$\theta \in [0,1]$

$\theta(\xi)$

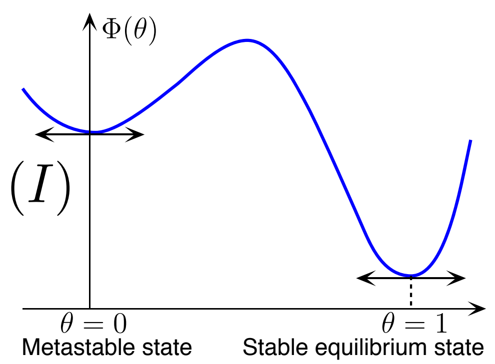
$\xi \equiv x + \mu t$

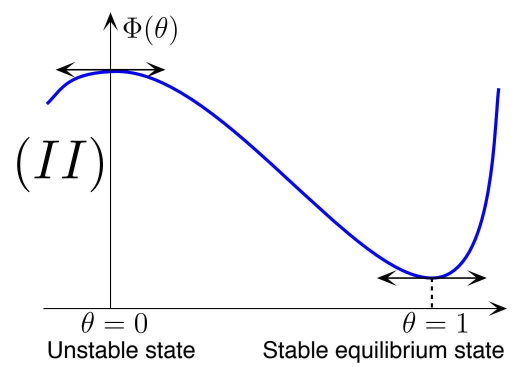
$\partial/\partial t = \mu\, \mathrm{d}/\mathrm{d}\xi$

$\partial/\partial x = \mathrm{d}/\mathrm{d}\xi$

μ is an eigenvalue of the problem
$$\mu\frac{\mathrm{d}\theta}{\mathrm{d}\xi} - \frac{\mathrm{d}^2\theta}{\mathrm{d}\xi^2} = w(\theta)$$

$\mathrm{d}\Phi/\mathrm{d}\theta = -w(\theta)$



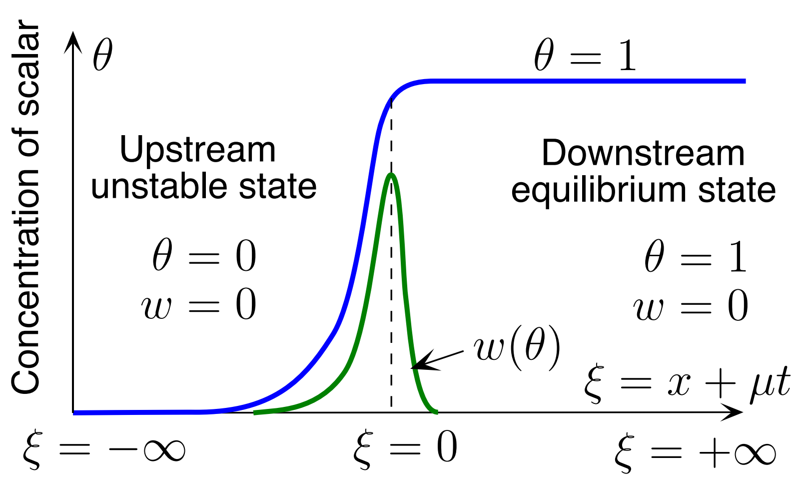


$\xi = -\infty: \quad \theta = 0,\ w = 0,$
initial state

$\xi = +\infty: \quad \theta = 1,\ w = 0$
final (equilibrium) state

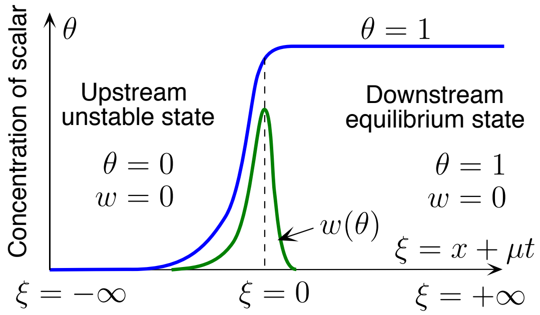
μ unknown, number of solutions ?

ZFK flame model: $\omega > 0$, case (II)



Number of solutions ? phase space, phase portrait

$$\theta \geqslant 0$$



second order system

$$X \equiv \theta, \qquad Y \equiv \mu \mathrm{d}\theta/\mathrm{d}\xi$$

$$\mu \frac{\mathrm{d}X}{\mathrm{d}\xi} - \frac{\mathrm{d}^2 X}{\mathrm{d}\xi^2} = \omega(X) \qquad \mu\,?$$

$$\mathrm{d}X/\mathrm{d}\xi = Y/\mu \qquad \mathrm{d}Y/\mathrm{d}\xi = \mu\,[Y - \omega(X)]$$

$$\mathrm{d}Y/\mathrm{d}X = \mu^2[Y - w(X)]/Y$$

Linearisation about $X = 0, Y = 0$, $\xi \to -\infty$ and $X = 1, Y = 0$ $\quad \omega'_\theta < 0$, $\xi \to \infty$ (equilibrium state)

fixed points: $\mathrm{d}X/\mathrm{d}\xi = \mathrm{d}Y/\mathrm{d}\xi = 0$

$Y = 0,\ \mathrm{d}Y/\mathrm{d}\xi = 0$

$\mathrm{d}Y/\mathrm{d}X = 0/0$

Two eigenvalues r_+ and r_- and two eigendvectors k_+ and k_-

$$\delta X = A_+ e^{\xi\, r_+} + A_- e^{\xi\, r_-}, \qquad \delta Y = k_+ A_+ e^{\xi\, r_+} + k_- A_- e^{\xi\, r_-}$$

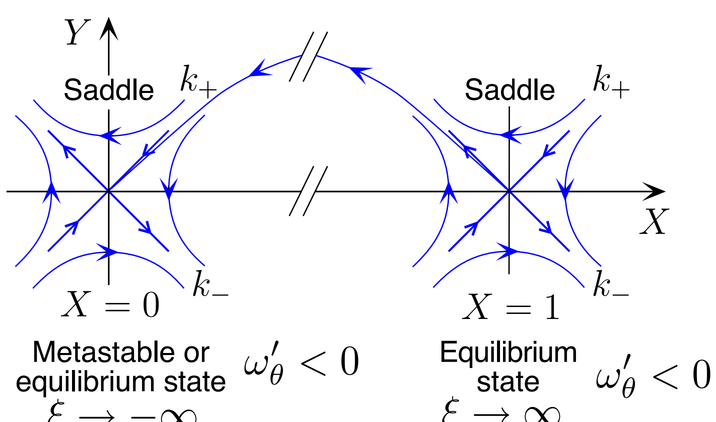
$$\mu \frac{\mathrm{d}\delta X}{\mathrm{d}\xi} - \frac{\mathrm{d}^2 \delta X}{\mathrm{d}\xi^2} = \omega'_\theta \delta X \qquad \mu r - r^2 - \omega'_\theta = 0$$

$$Y = \mu \frac{\mathrm{d}X}{\mathrm{d}\xi} \qquad \left[\frac{\mathrm{d}Y}{\mathrm{d}X}\right]_\pm = k_\pm$$

$$2r_\pm = \mu \pm \sqrt{\mu^2 - 4\omega'_\theta}$$

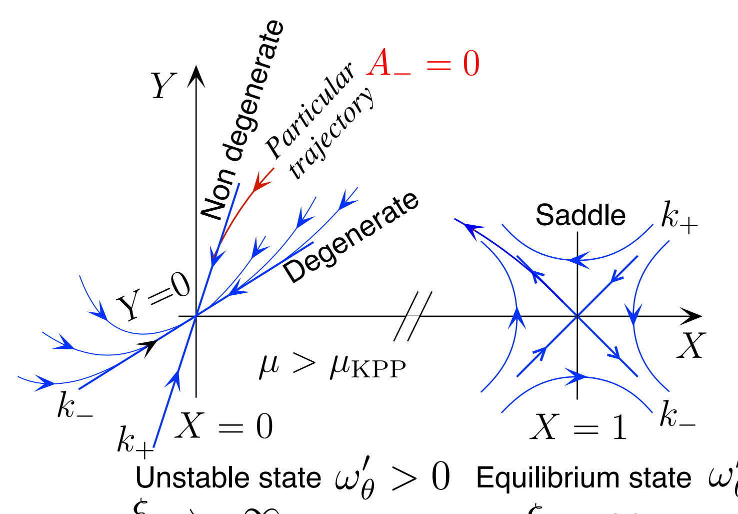
$$k_\pm = \mu r_\pm$$

case (I)



$r_- < 0,\ r_+ > 0 \qquad r_+ > 0,\ r_- < 0$

One solution

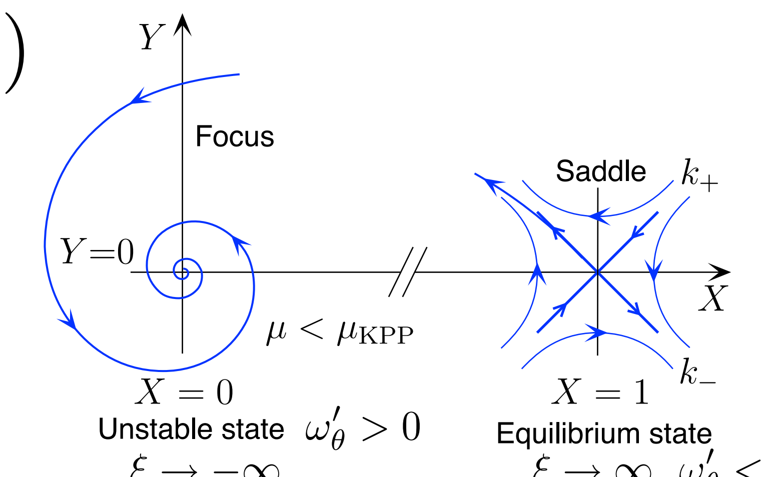


$r_+ > r_- > 0 \qquad r_+ > 0,\ r_- < 0$

Infinite numbers of solutions

One particular solution

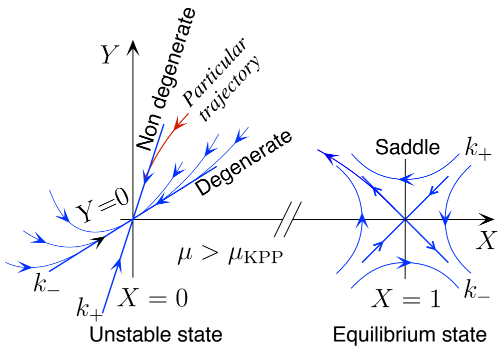
case (II)

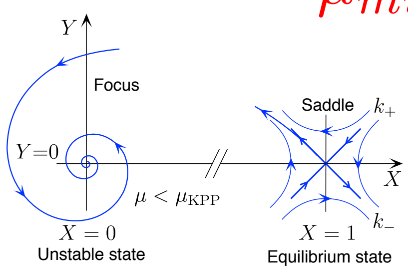


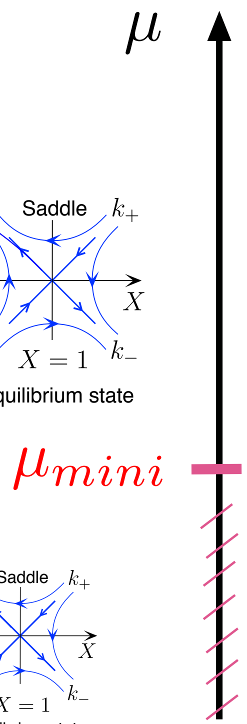
$\mathrm{Im}\, r_- \neq 0,\ \mathrm{Im}\, r_+ \neq 0\ \mathrm{Re}\, r_\pm > 0 \qquad r_+ > 0,\ r_- < 0$

No solution $(\theta \geqslant 0)$

Unstable medium







wave velocity

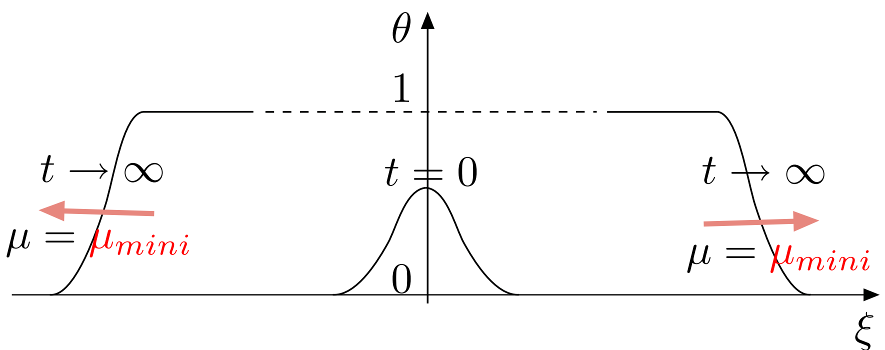
continuous spectrum with a lower bound

$$2r_\pm = \mu \pm \sqrt{\mu^2 - 4\omega'_\theta}$$

Kolmogorov 1937

$\mu_{mini} \equiv 2\sqrt{\mathrm{d}w/\mathrm{d}\theta|_{\theta=0}}$ lower bound : $r_+ = r_- = \mu/2$ $k_+ = k_-$

soft nonlinear term $\omega(\theta)$ soft case $\Rightarrow$ collapse of the 2 eigenvalues



the lower bound solution is selected $\mu_{mini} \equiv 2\sqrt{\mathrm{d}w/\mathrm{d}\theta|_{\theta=0}}$ $\neq$ $\mu_{\text{flame}} \propto \sqrt{2\int_0^1 w(\theta)\mathrm{d}\theta}$

$$\partial\theta/\partial t - \partial^2\theta/\partial\xi^2 = \omega'_o\theta, \quad \text{where} \quad \omega'_o \equiv \partial w/\partial\theta|_{\theta=0} > 0$$

$$\theta(\xi,t) \equiv Z(\xi,t)\mathrm{e}^{+\omega'_o t} \qquad \partial Z/\partial t - \partial^2 Z/\partial\xi^2 = 0$$

$$Z = \mathrm{e}^{-\xi^2/4t}/\sqrt{t} \qquad \theta \propto \exp[-\xi^2/4t + \omega'_o t - \ln(t)/2]$$

$\xi^2 \approx 4\omega'_o t^2$

OK for a soft term $\omega(\theta)$

Wrong for a stiff term $\omega(\theta)$

The lower bound solution changes of nature when $\omega(\theta)$ get stiffer

Clavin, Linan 1984

Soft $\omega(\theta) = \theta(1-\theta)$

Stiff $w(\theta,\beta) = (\beta^2/2)\theta(1-\theta)\mathrm{e}^{-\beta(1-\theta)}$, $\beta \gg 1$